R & D facts
U.S. Department of Energy
Office of Fossil Energy
National Energy Technology Laboratory

5/2006

Mercury Interaction with Large Aromatic Systems

Background

Mercury, a hazardous metal, exists in trace amounts in fossil fuels, vegetation, the earth's crust, and waste products. Power plants, municipal waste incinerators and other sources emit an estimated 5,000 tons of mercury each year into the atmosphere as vapor, which then can drift and spread over wide regions. Although mercury emissions decreased in the United States during the 1990s, researchers continue to seek new ways to remove mercury from flue gas more cost-effectively. The injection of activated carbon is one way to remove mercury from flue gas. The effectiveness of activated carbon depends on the characteristics of the fuel, temperature, flue gas components, and the amount of fly ash present. A high carbon-to-mercury ratio is needed to reduce mercury levels in the flue gas to acceptable levels. To improve the effectiveness of activated carbon as a method of mercury sorption, researchers must have a better understanding of the nature of the interaction between mercury and activated carbon.

Goals

Planned and ongoing research at NETL in the Computational Chemistry Group has the following goals:

- Conduct high-level quantum mechanical calculations on a series of aromatic molecules, starting with benzene, furan, and thiophene, to investigate the interactions of mercury with these aromatic molecules.
- Expand this work to larger polycyclic molecules, such as naphthalene, phenanthrene and coronene.
- Model the interaction of mercury with functionalized aromatic molecules such as 2-hydroxydibenzofuran; and
- Further expand the understanding of the interaction of mercury with extended and functionalized aromatic molecules.

Technical Approach

Little is known at the molecular level about the interaction of mercury with activated carbon. *Ab initio* methods can reveal detailed information at the molecular level about chemical and physical interactions. It would be impossible to use *ab initio* methods directly on activated carbon because these calculations are possible only

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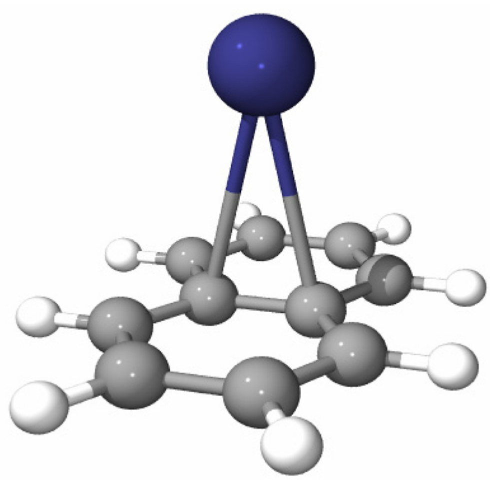
for a fairly small number of atoms, or for materials that have a regularly repeating structure, such as a crystal. Benzene and other aromatic molecules that are small enough to be modeled using *ab initio* methods can be employed as models for graphitic portions of activated carbon, because, as in graphite, the electrons in benzene are delocalized. Calculations involving aromatic molecules including functional groups can provide additional information by allowing researchers to quantify the strength of the chemical interactions possible between mercury and the functional groups present.

In this ongoing work, researchers are focusing on the interaction of mercury with naphthalene, as well as 2-hydroxydibenzofuran. The latter functionalized aromatic was selected because the hydroxide group is thought to play a role in the interaction between mercury and activated carbon.

Researchers at NETL have shown that neutral, ground state mercury forms a weakly bound complex with aromatic molecules such as benzene, furan and thiophene. The presence of the heteroatom in furan and thiophene makes little difference in the interaction of mercury with these aromatics. However, these complexes become strongly bound in the cationic state as well as in the triplet (excited) state. Preliminary calculations show that these conclusions are likely to be generalized for larger aromatic complexes such as naphthalene.

Benefits

- Yield information that leads to an understanding of how mercury interacts with the graphitic areas or functional groups present in activated carbon.
- Contribute to the future improvement of mercury sorbents, and
- Cost-effectively remove mercury from the flue gas of power plants.



(Hg-naphthalene)$^+$ minimum energy π complex. The complex is bound by -2.6 eV with respect to neutral naphthalene and the Hg^+ cation